

Ethylene oxide  
75-21-8 | DTXSID0020600

Model Performance

|       |      |
|-------|------|
| Model | Data |
|-------|------|

Weighted KNN model

| 5-fold CV (75%) |      | Training (75%) |      | Test (25%) |      |
|-----------------|------|----------------|------|------------|------|
| Q2              | RMSE | R2             | RMSE | R2         | RMSE |
| 0.81            | 0.55 | 0.81           | 0.54 | 0.71       | 0.61 |

Model Results

Predicted value: 3.03 L/kg

Global applicability domain: Inside

Local applicability domain index: 6.21e-01

Confidence level: 6.95e-01

Nearest Neighbors from the Training Set

|  |   |  |
|--|---|--|
| <div>Image not found</div> <div>Ethyleneimine</div> <div>Measured: 6.03</div> <div>Predicted: 4.17</div> | <div>Image not found</div> <div>Ethanol</div> <div>Measured: 1.58</div> <div>Predicted: 2.24</div>  | <div>Image not found</div> <div>Thioacetamide</div> <div>Measured: 6.03</div> <div>Predicted: 6.43</div> |
| <div>Image not found</div> <div>Acetic acid</div> <div>Measured: 1.00</div> <div>Predicted: 2.40</div>   | <div>Image not found</div> <div>Methanol</div> <div>Measured: 2.75</div> <div>Predicted: 2.76</div> |  |